WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Monday, March 19, 2007

Hide?	Set Name	Query	Hit Count
		DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ	
☐	L9	L8 and (atomic coordinates or diffract$5)	30
☐	L8	(dipeptidyl peptidase adj3 IV or dpp adj3 IV) and crystal and x-ray	68
		DB=PGPB; THES=ASSIGNEE; PLUR=YES; OP=ADJ	
☐	L7	L6 and (atomic coordinates or diffraction)	61
☐	L6	L5 and x-ray	148
☐	L5	L4 and crystal	514
☐	L4	(dipeptidyl peptidase adj3 IV or dpp adj3 IV)	1309
☐	L3	(dipeptidyl peptidase adj3 IV or dpp adj3 IV) and crystal and x-ray and difract$5	0
		DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ	
☐	L2	(dipeptidyl peptidase adj3 IV or dpp adj3 IV) and crystal and x-ray and difract$5	0
☐	L1	(dipeptidyl peptidase adj3 IV or dpp adj3 IV) and crystal and x-ray difract$5	0

END OF SEARCH HISTORY

FILE 'HOME' ENTERED AT 12:54:51 ON 19 MAR 2007

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=> file .nash
=> s (dipeptidyl peptidase(1w)IV or dpp(1w)IV) and crystal and x-ray
L1          18 FILE MEDLINE
L2          22 FILE CAPLUS
L3          19 FILE SCISEARCH
L4           1 FILE LIFESCI
L5          10 FILE BIOSIS
L6          13 FILE EMBASE

TOTAL FOR ALL FILES
L7          83 (DIPEPTIDYL PEPTIDASE(1W) IV OR DPP(1W) IV) AND CRYSTAL AND
               X-RAY

=> s l7 not 2003-2007/py
TOTAL FOR ALL FILES
L14          6 L7 NOT 2003-2007/PY

=> dup rem l14
PROCESSING COMPLETED FOR L14
L15          5 DUP REM L14 (1 DUPLICATE REMOVED)

=> d ibib abs 1-5

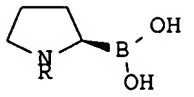
L15  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2001:723704  CAPLUS  Full-text
DOCUMENT NUMBER:         136:2627
TITLE:                   Sulphostin, a potent inhibitor for dipeptidyl
                         peptidase IV from Streptomyces sp.
                         MK251-43F3
AUTHOR(S):               Akiyama, Tetsuo; Abe, Masatoshi; Harada, Shigeko;
                         Kojima, Fukiko; Sawa, Ryuichi; Takahashi, Yoshikazu;
                         Naganawa, Hiroshi; Homma, Yoshiko; Hamada, Masa;
                         Yamaguchi, Akihito; Aoyagi, Takaaki; Muraoka,
                         Yasuhiko; Takeuchi, Tomio
CORPORATE SOURCE:        Institute of Microbial Chemistry, Tokyo, 141-0021,
                         Japan
SOURCE:                  Journal of Antibiotics (2001), 54(9), 744-746
                         CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER:               Japan Antibiotics Research Association
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB      The production, isolation, and structure elucidation of isolated sulfostin (1) and its epimer were
        presented.  Sulfostin was isolated from the culture broth of Streptomyces sp. MK251-43F3 together
        with its epimer, which was found to be formed during the isolation process.  The fermentation
        process of producing sulfostin was extremely hard due to low productivity, tedious isolation
        procedure, and unavoidable epimerization during the isolation process.  Chemical syntheses of
        sulfostin and its three diastereomers was successfully obtained.  The X-ray crystal anal. of
        synthesized 1 showed that the absolute configurations of the C-3 and the phosphorus atoms of 1
        were S and R, resp.  The structure of sulfostin was found to be 3(S)-amino-1-[(R)-
        amino(sulfoamino)phosphinyl]-2- piperidone.  Sulfostin showed inhibitory activities of dipeptidyl
        peptidase IV (DPPIV) with dose-dependent manner, and the IC50 value was 6 ng/mL, which was
        determined to be 100-fold stronger than that of diprotin A (a known DPP-IV inhibitor).
REFERENCE COUNT:         13    THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15  ANSWER 2 OF 5  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2000:752831  CAPLUS  Full-text
DOCUMENT NUMBER:         134:38982
TITLE:                   A novel free-mounting system for protein
                         crystals: transformation and improvement of
                         diffraction power by accurately controlled humidity
                         changes
AUTHOR(S):               Kiefersauer, Reiner; Than, Manuel E.; Dobbek, Holger;
                         Gremer, Lothar; Melero, Marcos; Strobl, Stefan; Dias,
                         Joao; Soulimane, Tewfik; Huber, Robert
CORPORATE SOURCE:        Max-Planck-Institut fur Biochemie, Martinsried,
                         D-82152, Germany
SOURCE:                  Journal of Applied Crystallography (2000), 33(5),
                         1223-1230
                         CODEN: JACGAR; ISSN: 0021-8898
PUBLISHER:               Munksgaard International Publishers Ltd.
```

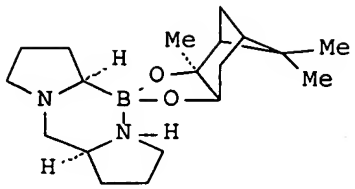
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel device for capillary-free mounting of protein crystals is described. A controlled stream of air allows an accurate adjustment of the humidity at the crystal. The crystal is held on the tip of a micropipette. With a video system (CCD camera), the two-dimensional shadow projections of crystals can be recorded for optical anal. Instead of the micropipette, a standard loop can also be used. Expts. and results for different crystal systems demonstrate the use of this method, also in combination with shock-freezing, to improve crystal order. Working with oxygen-free gases offers the possibility of crystal measurements under anaerobic conditions. Furthermore, the controlled application of arbitrary volatile substances with the gas stream is practicable.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 1998:78797 CAPLUS Full-text
DOCUMENT NUMBER: 128:254527
TITLE: Structure of proline iminopeptidase from Xanthomonas campestris pv. citri: a prototype for the prolyl oligopeptidase family
AUTHOR(S): Medrano, F. J.; Alonso, J.; Garcia, J. L.; Romero, A.; Bode, W.; Gomis-Ruth, F. X.
CORPORATE SOURCE: Max-Plank-Institut fur Biochemie, Abteilung Strukturforschung, Martinsried, D-82152, Germany
SOURCE: EMBO Journal (1998), 17(1), 1-9
CODEN: EMJODG; ISSN: 0261-4189
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Proline iminopeptidase (I) from X. campestris pv. citri is a serine peptidase that catalyzes the removal of N-terminal Pro residues from peptides with high specificity. Here, the authors solved its 3-dimensional structure by multiple isomorphous replacement and refined it to a crystallog. R-factor of 19.2% using x-ray data to 2.7 Å resolution I was folded into 2 contiguous domains. The larger domain showed the general topol. of the α/β hydrolase fold, with a central 8-stranded β-sheet flanked by 2 helixes and the 11 N-terminal residues on one side, and by 4 helixes on the other side. The smaller domain was placed on top of the larger domain and essentially consisted of 6 helixes. The active site, located at the end of a deep pocket at the interface between both domains, included a catalytic triad of Ser-110, Asp-266, and His-294. Cys-269, located at the bottom of the active site very close to the catalytic triad, presumably accounts for the inhibition by thiol-specific reagents. The overall topol. of I was very similar to that of yeast serine carboxypeptidase. The striking secondary structure similarity to human lymphocytic prolyl oligopeptidase and dipeptidyl peptidase IV makes this I structure a suitable model for the 3-dimensional structure of other peptidases of this family.
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:183432 CAPLUS Full-text
DOCUMENT NUMBER: 122:240402
TITLE: Studies on Proline Boronic Acid Dipeptide Inhibitors of Dipeptidyl Peptidase IV
: Identification of a Cyclic Species Containing a B-N Bond
AUTHOR(S): Snow, Roger J.; Bachovchin, William W.; Barton, Randall W.; Campbell, Scot J.; Coutts, Simon J.; Freeman, Dorothy M.; Gutheil, William G.; Kelly, Terence A.; Kennedy, Charles A.; et al.
CORPORATE SOURCE: Department of Medicinal Chemistry Pharmacology, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Journal of the American Chemical Society (1994), 116(24), 10860-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB The proline boronic acid dipeptides I (R = H-Ala, H-Pro, H-Val) are very potent inhibitors of the enzyme dipeptidyl peptidase IV (DPP IV or CD26), found on the surface of T-cells, and are a new class of immunosuppressants. The efficient synthesis of the free boronic acids as single enantiomers is described, and the absolute configuration determined I lose DPP IV inhibitory activity in solution: this is shown to be due to the reversible formation of a cyclic species analogous to a diketopiperazine, containing a B-N bond. The cyclic compds., both as the free boronic acids and as the pinanediol esters, were isolated and characterized by 1H and 11B NMR, and in the case of II, by x-ray crystallog. The cyclization is pH dependent, with the open form favored at low pH, while the cyclic form predominates at neutral pH. Both the rate and extent of cyclization depend on the N-terminal amino acid. The rates of cyclization have been measured by 1H NMR and shown to correlate with the decrease in DPP IV inhibitory activity. I (R = H-Val) cyclizes more slowly, and to a lesser extent than I (R = H-Ala, H-Pro), which is predicted to lead to greater immunosuppressive potency in vivo.

L15 ANSWER 5 OF 5 EMBASE COPYRIGHT (c) 2007 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 74010061 EMBASE Full-text
DOCUMENT NUMBER: 1974010061
TITLE: Chemical studies on tuberactinomycin. V. Structures of guanidino amino acids in tuberactinomycins.
AUTHOR: Wakamiya T.; Shiba T.; Kaneko T.; et al.
CORPORATE SOURCE: Dept. Chem., Fac. Sci., Osaka Univ., Toyonaka, Osaka, Japan
SOURCE: Bulletin of the Chemical Society of Japan, (1973) Vol. 46, No. 3, pp. 949-954. .
CODEN: BCSJA8
DOCUMENT TYPE: Journal
FILE SEGMENT: 037 Drug Literature Index
LANGUAGE: English
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

=> s (dipeptidyl peptidase(1w)IV or dpp(1w)IV) and crystal
L16 29 FILE MEDLINE
L17 63 FILE CAPLUS
L18 70 FILE SCISEARCH
L19 2 FILE LIFESCI
L20 28 FILE BIOSIS
L21 33 FILE EMBASE

TOTAL FOR ALL FILES
L22 225 (DIPEPTIDYL PEPTIDASE(1W) IV OR DPP(1W) IV) AND CRYSTAL

=> s l22 not 2003-2007/py
L23 2 FILE MEDLINE
L24 7 FILE CAPLUS
L25 6 FILE SCISEARCH
L26 0 FILE LIFESCI
L27 2 FILE BIOSIS
L28 4 FILE EMBASE

TOTAL FOR ALL FILES
L29 21 L22 NOT 2003-2007/PY

=> dup rem l29
PROCESSING COMPLETED FOR L29
L30 12 DUP REM L29 (9 DUPLICATES REMOVED)

=> d ibib abs 1-12

L30 ANSWER 1 OF 12 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2002:292458 SCISEARCH Full-text
THE GENUINE ARTICLE: 536GE
TITLE: Extracellular cysteines define ectopeptidase (APN, CD 13) expression and function
AUTHOR: Firla B (Reprint); Arndt M; Frank K; Thiel U; Ansorge S; Tager M; Lendeckel U
CORPORATE SOURCE: Univ Magdeburg, Inst Immunol, Leipziger Str 44, D-39120 Magdeburg, Germany (Reprint); Univ Magdeburg, Inst Immunol, D-39120 Magdeburg, Germany; Univ Magdeburg, Inst Expt Internal Med, Ctr Internal Med, D-39120 Magdeburg, Germany
COUNTRY OF AUTHOR: Germany
SOURCE: FREE RADICAL BIOLOGY AND MEDICINE, (1 APR 2002) Vol. 32, No. 7, pp. 584-595.
ISSN: 0891-5849.
PUBLISHER: PERGAMON-ELSEVIER SCIENCE LTD, THE BOULEVARD, LANGFORD LANE, KIDLINGTON, OXFORD OX5 1GB, ENGLAND.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 56
ENTRY DATE: Entered STN: 19 Apr 2002
Last Updated on STN: 19 Apr 2002
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Alanyl aminopeptidase (APN) is a surface-bound metallopeptidase that processes the N-terminals of biologically active peptides such as enkephalins, angiotensins, neurokinins, and cytokines. It exerts profound activity on vital processes such as immune response, cellular growth, and blood pressure control. Inhibition of either APN gene expression or its enzymatic activity severely affects leukocyte growth and function. We show here that oxidoreductase-mediated modulations of the cell surface thiol status affect the enzymatic activity of APN. Additional evidence for the pivotal role of extracellular cysteines in the APN molecule was obtained when substitution of any of these six cysteines caused complete loss of surface expression and enzymatic activity. In contrast, the transmembrane Cys24 appears to have no similar function. Enzymatically inactive cysteine mutants were retained in the endoplasmic reticulum as shown by high-resolution imaging and Endoglycosidase H digestion. In the absence of any crystal-structure data, the demonstration that individual extracellular cysteines contribute to APN expression and function appears to be of particular importance. The data are the first to show thiol-dependent modulation of the activity of a typical surface-bound peptidase at the cell surface, probably reflecting a general regulating mechanism. This may relate to various disease processes such as inflammation or malignant transformation, (C) 2002 Elsevier Science Inc.

L30 ANSWER 2 OF 12 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2002184012 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 11915948
TITLE: The prolyl oligopeptidase family.
AUTHOR: Polgar L
CORPORATE SOURCE: Institute of Enzymology, Hungarian Academy of Sciences, Budapest.
SOURCE: Cellular and molecular life sciences : CMLS, (2002 Feb) Vol. 59, No. 2, pp. 349-62. Ref: 156
Journal code: 9705402. ISSN: 1420-682X.
PUB. COUNTRY: Switzerland
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
General Review; (REVIEW)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200204
ENTRY DATE: Entered STN: 3 Apr 2002
Last Updated on STN: 13 Apr 2002
Entered Medline: 12 Apr 2002

AB A group of serine peptidases, the prolyl oligopeptidase family, cannot hydrolyze peptides containing more than about 30 residues. This group is unrelated to the classical trypsin and subtilisin families, and includes dipeptidyl peptidase IV, acylaminoacyl peptidase and oligopeptidase B, in addition to the prototype prolyl oligopeptidase. The recent crystal structure determination of prolyl oligopeptidase (80 kDa) has shown that the enzyme contains a peptidase domain with an alpha/beta hydrolase fold, and its catalytic triad is covered by the central tunnel of an unusual seven-bladed beta-propeller. This domain operates as a gating filter, excluding large, structured peptides from the active site. The binding mode of substrates and the catalytic mechanism differ from that of the classical serine peptidases in several features. The members of the family are important targets of drug design. Prolyl oligopeptidase

is involved in amnesia, depression and blood pressure control, dipeptidyl peptidase IV in type 2 diabetes and oligopeptidase B in trypanosomiasis.

L30 ANSWER 3 OF 12 EMBASE COPYRIGHT (c) 2007 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2003401962 EMBASE Full-text
TITLE: Proteolytic enzymes as therapeutic targets - Keystone symposium: 3-8 February 2002, Keystone, CO, USA.
AUTHOR: Creemers J.
CORPORATE SOURCE: J. Creemers, Department for Human Genetics, Katholieke Universiteit Leuven, Gasthuisberg O/N 6, Herestraat 49, B-3000 Leuven, Belgium. john.creemers@med.kuleuven.ac.be
SOURCE: IDrugs, (2002) Vol. 5, No. 3, pp. 216-219. .
ISSN: 1369-7056 CODEN: IDRUFN
COUNTRY: United Kingdom
DOCUMENT TYPE: Journal; Conference Article
FILE SEGMENT: 029 Clinical Biochemistry
037 Drug Literature Index
030 Pharmacology
003 Endocrinology
016 Cancer
033 Orthopedic Surgery
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 23 Oct 2003
Last Updated on STN: 23 Oct 2003

AB The Keystone Symposium 'Proteolytic Enzymes as Therapeutic Targets' was attended by approximately 150 scientists. Around two-thirds of the participants consisted of representatives from pharmaceutical companies, but representatives from academic institutes dominated the list of speakers. The meeting attracted scientists from many different fields, including biochemistry, molecular biology, structural biology, pharmacology, chemistry, and bioinformatics. The science ranged from the discovery and characterization of novel proteinases to the development and clinical trials of proteinase inhibitors and was presented as posters or in oral sessions. The discussions following the oral presentations were always very animated, but hardly ever heated. Although there were a few new drugs being presented, the real highlight was the enormous potential of recently discovered proteinases as new therapeutic targets. Both pharmaceutical companies and academic institutes are investing in programs to integrate the avalanche of new information coming from functional genomics, proteomics and structural information to create a platform for applied proteinase technology.

L30 ANSWER 4 OF 12 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2002:302127 SCISEARCH Full-text
THE GENUINE ARTICLE: 536QM
TITLE: Threading with chemostructural restrictions method for predicting fold and functionally significant residues: Application to dipeptidylpeptidase IV (DPP-IV)
AUTHOR: Reva B (Reprint); Finkelstein A; Topiol S
CORPORATE SOURCE: Discovery Partners Int, Computat Div, Suite 645, 2 Execut Dr, Ft Lee, NJ 07024 USA (Reprint); Novartis Inst Biomed Res, Summit, NJ USA; Russian Acad Sci, Inst Prot Res, Pushchino 142292, Moscow Region, Russia
COUNTRY OF AUTHOR: USA; Russia
SOURCE: PROTEINS-STRUCTURE FUNCTION AND GENETICS, (1 MAY 2002) Vol. 47, No. 2, pp. 180-193.
ISSN: 0887-3585.
PUBLISHER: WILEY-LISS, DIV JOHN WILEY & SONS INC, 605 THIRD AVE, NEW YORK, NY 10158-0012 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 52
ENTRY DATE: Entered STN: 19 Apr 2002
Last Updated on STN: 19 Apr 2002
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB We present a new method for more accurate modeling of protein structure, called threading with chemostructural restrictions. This method addresses those cases in which a target sequence has only remote homologues of known structure for which sequence comparison methods cannot provide accurate alignments. Although remote homologues cannot provide an accurate model for the whole chain, they can be used in constructing practically useful models for the most conserved-and often the most interesting-part of the structure. For many proteins of interest, one can suggest certain chemostructural patterns for the native structure based on the available information on the structural superfamily of the protein,

the type of activity, the sequence location of the functionally significant residues, and other factors. We use such patterns to restrict (1) a number of possible templates, and (2) a number of allowed chain conformations on a template. The latter restrictions are imposed in the form of additional template potentials (including terms acting as sequence anchors) that act on certain residues. This approach is tested on remote homologues of alpha/beta-hydrolases that have significant structural similarity in the positions of their catalytic triads. The study shows that, in spite of significant deviations between the model and the native structures, the surroundings of the catalytic triad (positions of C-alpha atoms of 20-30 nearby residues) can be reproduced with accuracy of 2-3 Angstrom. We then apply the approach to predict the structure of dipeptidylpeptidase IV (DPP-IV). Using experimentally available data identifying the catalytic triad residues of DPP- IV (David et al., J Biol Chem 1993;268:1724717252); we predict a model structure of the catalytic domain of DPP-TV based on the 3D fold of prolyl oligopeptidase (Fulop et al., Cell 1998;94:161-170) and use this structure for modeling the interaction of DPP-IV with inhibitor.

L30 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:723704 CAPLUS Full-text
DOCUMENT NUMBER: 136:2627
TITLE: Sulphostin, a potent inhibitor for dipeptidyl peptidase IV from Streptomyces sp. MK251-43F3
AUTHOR(S): Akiyama, Tetsuo; Abe, Masatoshi; Harada, Shigeko; Kojima, Fukiko; Sawa, Ryuichi; Takahashi, Yoshikazu; Naganawa, Hiroshi; Homma, Yoshiko; Hamada, Masa; Yamaguchi, Akihito; Aoyagi, Takaaki; Muraoka, Yasuhiko; Takeuchi, Tomio
CORPORATE SOURCE: Institute of Microbial Chemistry, Tokyo, 141-0021, Japan
SOURCE: Journal of Antibiotics (2001), 54(9), 744-746
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The production, isolation, and structure elucidation of isolated sulfostin (1) and its epimer were presented. Sulfostin was isolated from the culture broth of Streptomyces sp. MK251-43F3 together with its epimer, which was found to be formed during the isolation process. The fermentation process of producing sulfostin was extremely hard due to low productivity, tedious isolation procedure, and unavoidable epimerization during the isolation process. Chemical syntheses of sulfostin and its three diastereomers was successfully obtained. The X-ray crystal anal. of synthesized 1 showed that the absolute configurations of the C-3 and the phosphorus atoms of 1 were S and R, resp. The structure of sulfostin was found to be 3(S)-amino-1-[(R)-amino(sulfoamino)phosphinyl]-2-piperidone. Sulfostin showed inhibitory activities of dipeptidyl peptidase IV (DPPIV) with dose-dependent manner, and the IC50 value was 6 ng/mL, which was determined to be 100-fold stronger than that of diprotin A (a known DPP-IV inhibitor).
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:752831 CAPLUS Full-text
DOCUMENT NUMBER: 134:38982
TITLE: A novel free-mounting system for protein crystals: transformation and improvement of diffraction power by accurately controlled humidity changes
AUTHOR(S): Kiefersauer, Reiner; Than, Manuel E.; Dobbek, Holger; Gremer, Lothar; Melero, Marcos; Strobl, Stefan; Dias, Joao; Soulimane, Tewfik; Huber, Robert
CORPORATE SOURCE: Max-Planck-Institut fur Biochemie, Martinsried, D-82152, Germany
SOURCE: Journal of Applied Crystallography (2000), 33(5), 1223-1230
CODEN: JACGAR; ISSN: 0021-8898
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel device for capillary-free mounting of protein crystals is described. A controlled stream of air allows an accurate adjustment of the humidity at the crystal. The crystal is held on the tip of a micropipette. With a video system (CCD camera), the two-dimensional shadow projections of crystals can be recorded for optical anal. Instead of the micropipette, a standard loop can also be used. Expts. and results for different crystal systems demonstrate the use of this method, also in combination with shock-freezing, to improve crystal order. Working with oxygen-free gases offers the possibility of crystal measurements under anaerobic conditions. Furthermore, the controlled application of arbitrary volatile substances with the gas stream is practicable.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 12 MEDLINE on STN DUPLICATE 2
ACCESSION NUMBER: 2000181799 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 10716680
TITLE: Butyrate and trichostatin A effects on the proliferation/differentiation of human intestinal epithelial cells: induction of cyclin D3 and p21 expression.
AUTHOR: Siavoshian S; Segain J P; Kornprobst M; Bonnet C; Cherbut C; Galmiche J P; Blottiere H M
CORPORATE SOURCE: Centre de Recherche en Nutrition Humaine de Nantes, INSERM U539, CHU Hotel-Dieu, Nantes, France.
SOURCE: Gut, (2000 Apr) Vol. 46, No. 4, pp. 507-14.
Journal code: 2985108R. ISSN: 0017-5749.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: (COMPARATIVE STUDY)
Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Abridged Index Medicus Journals; Priority Journals
ENTRY MONTH: 200004
ENTRY DATE: Entered STN: 12 May 2000
Last Updated on STN: 12 May 2000
Entered Medline: 28 Apr 2000

AB BACKGROUND: Sodium butyrate, a product of colonic bacterial fermentation, is able to inhibit cell proliferation and to stimulate cell differentiation of colonic epithelial cell lines. It has been proposed that these cellular effects could be linked to its ability to cause hyperacetylation of histone through the inhibition of histone deacetylase. AIM: To analyse the molecular mechanisms of butyrate action on cell proliferation/differentiation and to compare them with those of trichostatin A, a well known inhibitor of histone deacetylase. METHODS: HT-29 cells were grown in the absence or presence of butyrate or trichostatin A. Cell proliferation and cell cycle distribution were studied after DNA staining by crystal violet and propidium iodide respectively. Cell cycle regulatory proteins were studied by western blot and reverse transcription-polymerase chain reaction. Cell differentiation was followed by measuring brush border enzyme activities. Histone acetylation was studied by acid/urea/Triton acrylamide gel electrophoresis. RESULTS: Butyrate blocked cells mainly in the G(1) phase of the cell cycle, whereas trichostatin A was inhibitory in both G(1) and G(2) phases. Butyrate inhibited the mRNA expression of cyclin D1 without affecting its protein expression and stimulated the protein expression of cyclin D3 without affecting its mRNA expression. Trichostatin A showed similar effects on cyclin D1 and D3. Butyrate and trichostatin A stimulated p21 expression both at the mRNA and protein levels, whereas their effects on the expression of cyclin dependent kinases were slightly different. Moreover, butyrate strongly stimulated the activity of alkaline phosphatase and dipeptidyl peptidase IV, whereas trichostatin A had no effect. Finally, a six hour exposure to butyrate or trichostatin A induced histone H4 hyperacetylation. At 15 and 24 hours, histone H4 remained hyperacetylated in the presence of butyrate, whereas it returned to control levels in the presence of trichostatin A. CONCLUSIONS: The data may explain how butyrate acts on cell proliferation/differentiation, and they show that trichostatin A does not reproduce every effect of butyrate, mainly because of its shorter half life.

L30 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:765555 CAPLUS Full-text
DOCUMENT NUMBER: 130:133643
TITLE: Inhibition of dipeptidyl peptidase IV by fluoroolefin-containing N-peptidyl-O-hydroxylamine peptidomimetics
AUTHOR(S): Lin, Jian; Toscano, Paul J.; Welch, John T.
CORPORATE SOURCE: Department of Chemistry, University at Albany, Albany, NY, 12222, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1998), 95(24), 14020-14024
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dipeptidyl peptidase IV (EC 3.4.14.5; DPP IV), also known as the leukocyte differentiation antigen CD26 when found as an extracellular membrane-bound proline specific serine protease, cleaves a dipeptide from the N terminus of a polypeptide chain containing a proline residue in the penultimate position. Here the authors report that known (Z)-Ala-ψ[CF=C]-Pro dipeptide isosteres, which contain O-acylhydroxylamines, were isolated as diastereomeric pairs. The effect of each diastereomeric pair as an inhibitor of human placental dipeptidyl peptidase DPP IV has been examined The inhibition of DPP IV by these compds. is rapid and efficient. Fluoroolefin containing N-peptidyl-O-hydroxylamine peptidomimetics, by virtue of their inhibitory potency and

stability, are superior to N-peptidyl-O-hydroxylamine inhibitors derived from an Ala-Pro dipeptide.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 1998:78797 CAPLUS Full-text

DOCUMENT NUMBER: 128:254527

TITLE: Structure of proline iminopeptidase from Xanthomonas campestris pv. citri: a prototype for the prolyl oligopeptidase family

AUTHOR(S): Medrano, F. J.; Alonso, J.; Garcia, J. L.; Romero, A.; Bode, W.; Gomis-Ruth, F. X.

CORPORATE SOURCE: Max-Plank-Institut fur Biochemie, Abteilung Strukturforschung, Martinsried, D-82152, Germany

SOURCE: EMBO Journal (1998), 17(1), 1-9
CODEN: EMJODG; ISSN: 0261-4189

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Proline iminopeptidase (I) from X. campestris pv. citri is a serine peptidase that catalyzes the removal of N-terminal Pro residues from peptides with high specificity. Here, the authors solved its 3-dimensional structure by multiple isomorphous replacement and refined it to a crystallog. R-factor of 19.2% using x-ray data to 2.7 Å resolution I was folded into 2 contiguous domains. The larger domain showed the general topol. of the α/β hydrolase fold, with a central 8-stranded β-sheet flanked by 2 helixes and the 11 N-terminal residues on one side, and by 4 helixes on the other side. The smaller domain was placed on top of the larger domain and essentially consisted of 6 helixes. The active site, located at the end of a deep pocket at the interface between both domains, included a catalytic triad of Ser-110, Asp-266, and His-294. Cys-269, located at the bottom of the active site very close to the catalytic triad, presumably accounts for the inhibition by thiol-specific reagents. The overall topol. of I was very similar to that of yeast serine carboxypeptidase. The striking secondary structure similarity to human lymphocytic prolyl oligopeptidase and dipeptidyl peptidase IV makes this I structure a suitable model for the 3-dimensional structure of other peptidases of this family.

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:183432 CAPLUS Full-text

DOCUMENT NUMBER: 122:240402

TITLE: Studies on Proline Boronic Acid Dipeptide Inhibitors of Dipeptidyl Peptidase IV
: Identification of a Cyclic Species Containing a B-N Bond

AUTHOR(S): Snow, Roger J.; Bachovchin, William W.; Barton, Randall W.; Campbell, Scot J.; Coutts, Simon J.; Freeman, Dorothy M.; Gutheil, William G.; Kelly, Terence A.; Kennedy, Charles A.; et al.

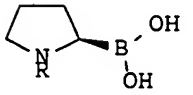
CORPORATE SOURCE: Department of Medicinal Chemistry Pharmacology, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA

SOURCE: Journal of the American Chemical Society (1994), 116(24), 10860-9
CODEN: JACSAT; ISSN: 0002-7863

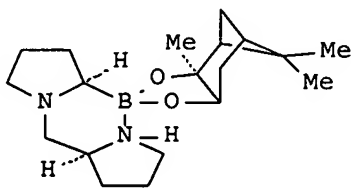
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The proline boronic acid dipeptides I (R = H-Ala, H-Pro, H-Val) are very potent inhibitors of the enzyme dipeptidyl peptidase IV (DPP IV or CD26), found on the surface of T-cells, and are a new class of immunosuppressants. The efficient synthesis of the free boronic acids as single enantiomers is described, and the absolute configuration determined I lose DPP IV inhibitory activity in solution: this is shown to be due to the reversible formation of a cyclic species analogous to a diketopiperazine, containing a B-N bond. The cyclic compds., both as the free boronic acids and as the pinanediol esters, were isolated and characterized by 1H and 11B NMR, and in the case of II, by x-ray crystallog. The cyclization is pH dependent, with the open form favored at low pH, while the cyclic form predominates at neutral pH. Both the rate and extent of cyclization depend on the N-terminal amino acid. The rates of cyclization have been measured by 1H NMR and shown to correlate with the decrease in DPP IV inhibitory activity. I (R = H-Val) cyclizes more slowly, and to a lesser extent than I (R = H-Ala, H-Pro), which is predicted to lead to greater immunosuppressive potency in vivo.

L30 ANSWER 11 OF 12 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1994:217981 SCISEARCH Full-text
THE GENUINE ARTICLE: NF042
TITLE: INFLUENCE ON PROLINE-SPECIFIC ENZYMES OF A SUBSTRATE CONTAINING THE THIOXOAMINOACYL-PROLYL PEPTIDE-BOND
AUTHOR: SCHUTKOWSKI M (Reprint); NEUBERT K; FISCHER G
CORPORATE SOURCE: MAX PLANCK GESELL FORDERUNG WISSENSCH EV, ARBEITSGRP ENZYMOL PEPTIDBINDUNG, WEINBERGWEG 16A, D-06120 HALLE, GERMANY (Reprint); UNIV HALLE WITTENBERG, INST BIOCHEM, FACHBEREICH BIOCHEM BIOTECHNOL, HALLE, GERMANY
COUNTRY OF AUTHOR: GERMANY
SOURCE: EUROPEAN JOURNAL OF BIOCHEMISTRY, (1 APR 1994) Vol. 221, No. 1, pp. 455-461.
ISSN: 0014-2956.
PUBLISHER: SPRINGER VERLAG, 175 FIFTH AVE, NEW YORK, NY 10010.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: LIFE
LANGUAGE: English
REFERENCE COUNT: 57
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Dipeptidyl peptidase IV from porcine kidney and aminopeptidase P from Escherichia coli can utilize thioxoalanyl-proline 4-nitroanilide but with decreased kinetic constants compared to the nor mal substrates. Product analysis showed that exclusively thioxoalanyl-proline was liberated in the case of dipeptidyl peptidase IV catalysis and thioxo-alanine in the case of aminopeptidase-P-mediated thioxo peptide bond hydrolysis. For the proline-specific aminopeptidase P the k(cat)/K-m value for the thioxo peptide is 1100-fold lower than for the corresponding oxo peptide. This difference is entirely due to k(cat). Because the rotation about the thioxo amide bond is about 12.5 kJ mol(-1) more difficult than rotation about an amide bond, these data support a mechanism involving rate-limiting rotation about the scissile peptide bond. It was found that the specificity rate constant for the reaction of thioxoalanyl-proline LF-nitroanilide and dipeptidyl peptidase TV is 100-1000-fold lower compared to the corresponding rate constant for alanyl-proline 4-nitroanilide. This remarkable effect is interpreted in terms of a distorted binding of the transition state for the thioxo substrate. The hydrolysis of the thioxo substrate by dipeptidyl peptidase IV is isomer-specific. The conformation about the nonscissile P-2-P-1 thioxo amide bond has to be in trans for successful cleavage of the scissile peptide bond. We can now directly compare the rotational energy barrier of the prolyl peptide bond for the oxo and the thioxo form.

L30 ANSWER 12 OF 12 EMBASE COPYRIGHT (c) 2007 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 74010061 EMBASE Full-text
DOCUMENT NUMBER: 1974010061
TITLE: Chemical studies on tuberactinomycin. V. Structures of guanidino amino acids in tuberactinomycins.
AUTHOR: Wakamiya T.; Shiba T.; Kaneko T.; et al.
CORPORATE SOURCE: Dept. Chem., Fac. Sci., Osaka Univ., Toyonaka, Osaka, Japan
SOURCE: Bulletin of the Chemical Society of Japan, (1973) Vol. 46, No. 3, pp. 949-954.
CODEN: BCSJA8
DOCUMENT TYPE: Journal
FILE SEGMENT: 037 Drug Literature Index
LANGUAGE: English
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

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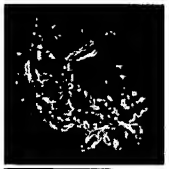
☑ **2BUB**



CRYSTAL STRUCTURE OF HUMAN DIPEPTIDYL PEPTIDASE IV (CD26) IN COMPLEX WITH A REVERSED AMIDE INHIBITOR

Characteristics **Release Date:** 23-Jan-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.66 Å

Classification **Complex (hydrolase/inhibitor)**

Compound Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE 4 Fragment: EXTRACELLULAR DOMAIN, RESIDUES 39-766 Chains: A,B EC no.: 3.4.14.5

Authors **Nordhoff, S., Cerezo-Galvez, S., Feurer, A., Hill, O., Matassa, V.G., Metz, G., Rummey, C., Thiemann, M., Edwards, P.J.**

☑ **1U7F**

Crystal Structure of the phosphorylated Smad3/Smad4 heterotrimeric complex

Characteristics **Release Date:** 28-Sep-2004 **Exp. Method:** X Ray Diffraction
Resolution: 2.60 Å

Classification **Signaling Protein**

Compound Polymer: 1 Molecule: Mothers against decapentaplegic homolog 3 Fragment: MH2 and Linker domains Chains: A,C
Polymer: 2 Molecule: Mothers against decapentaplegic homolog 4 Fragment: MH2 and Linker domains Chains: B

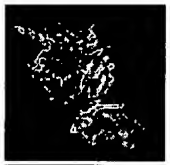
Authors **Chacko, B.M., Qin, B.Y., Tiwari, A., Shi, G., Lam, S., Hayward, L.J., De Caestecker, M., Lin,**

☑ **1U7V**

Crystal Structure of the phosphorylated Smad2/Smad4 heterotrimeric complex

Characteristics **Release Date:** 28-Sep-2004 **Exp. Method:** X Ray Diffraction
Resolution: 2.70 Å

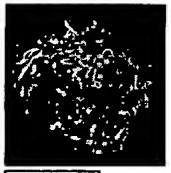
Classification **Signaling Protein**



Compound Polymer: 1 Molecule: Mothers against decapentaplegic homolog 2 Fragment: MH2 and Linker domains Chains: A,C
Polymer: 2 Molecule: Mothers against decapentaplegic homolog 4 Fragment: MH2 and Linker domains Chains: B

Authors **Chacko, B.M., Qin, B.Y., Tiwari, A., Shi, G., Lam, S., Hayward, L.J., De Caestecker, M., Lin,**

☑ **2GBC** **Native DPP-IV (CD26) from Rat**



Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.80 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Chains: A,B EC no.: 3.4.15.5

Authors **Longenecker, K.L., Stewart, K.D., Madar, D.J., Jakob, C.G., Fry, E.H., Wilk, S., Lin, C.W., Ballaron, S.J., Stashko, M.A., Lubben, T.H., Yong, H., Pireh, D., Pei, Z., Basha, F., Wiedeman, P.E., Von Geldern, T.W., Trevillyan, J.M., Stoll, V.S.**

☑ **1OZJ** **Crystal structure of Smad3-MH1 bound to DNA at 2.4 A resolution**

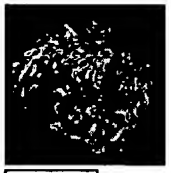
Characteristics **Release Date:** 23-Mar-2004 **Exp. Method:** X Ray Diffraction
Resolution: 2.40 Å

Classification **Transcription/dna**

Compound Polymer: 1 Molecule: Smad binding element Chains: C
Polymer: 2 Molecule: Smad binding element Chains: D
Polymer: 3 Molecule: SMAD 3 Fragment: DWA DOMAIN Chains: A,B

Authors **Chai, J., Wu, J.-W., Yan, N., Massague, J., Pavletich, N.P., Shi, Y.**

☑ **2GBI** **rat DPP-IV with xanthine inhibitor 4**



Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction
Resolution: 3.30 Å

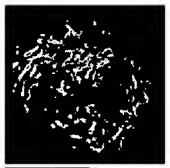
Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl Peptidase Soluble Form (residues 38-767) Chains: A,B EC no.: 3.4.14.5

Authors **Longenecker, K.L., Stewart, K.D., Madar, D.J., Jakob, C.G., Fry, E.H., Wilk, S., Lin, C.W., Ballaron, S.J., Stashko, M.A., Lubben, T.H., Yong, H., Pireh, D., Pei, Z., Basha,**

F., Wiedeman, P.E., Von Geldern, T.W., Trevillyan, J.M., Stoll, V.S.

☑ 2I3Z



rat DPP-IV with xanthine mimetic inhibitor #7

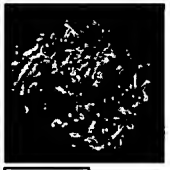
Characteristics **Release Date:** 12-Dec-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.90 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) Fragment: DIPEPTIDYL PEPTIDASE SOLUBLE FORM (RESIDUES 38-767) Chains: A,B EC no.: 3.4.14.5

Authors **Kurukulasuriya, R., Rohde, J.J., Szczepankiewicz, B.G., Basha, F., Lai, C., Jae, H.S., Winn, M., Stewart, K.D., Longenecker, K.L., Lubben, T.W., Ballaron, S.J., Sham, H.L., von Gelder T.W.**

☑ 2GBG



rat DPP-IV with alkynyl cyanopyrrolidine #2

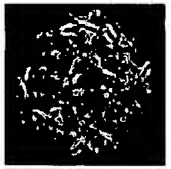
Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction
Resolution: 3.00 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl Peptidase 4 Soluble Form (Resid 38-767) Chains: A,B EC no.: 3.4.14.5

Authors **Longenecker, K.L., Stewart, K.D., Madar, D.J., Jakob, C.G., Fry, E.H., Wilk, S., Lin, C.W., Ballaron, S.J., Stashko, M.A., Lubben, T.H., Yong, H., Pireh, D., Pei, Z., Basha, F., Wiedeman, P.E., Von Geldern, T.W., Trevillyan, J.M., Stoll, V.S.**

☑ 1RWQ



Human Dipeptidyl peptidase IV in complex with 5-aminomethyl-6-(2,4-dichloro-phenyl)-2-(3,5-dimethoxy-phenyl)-pyrimidin-4-ylamine

Characteristics **Release Date:** 17-Dec-2004 **Exp. Method:** X Ray Diffraction
Resolution: 2.20 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase IV Chains: A,B EC no.: 3.4.14.5

Authors **Peters, J.U., Weber, S., Kritter, S., Weiss, P., Wallier, A., Boehringer, M., Hennig, M., Kuh B., Loeffler, B.M.**

☑ 1NU6

Crystal structure of human Dipeptidyl Peptidase IV (DPP-IV)

Characteristics	**Release Date:** 26-Aug-2003 **Exp. Method:** X Ray Diffraction **Resolution:** 2.10 Å
Classification	**Hydrolase**
Compound	Polymer: 1 Molecule: Dipeptidyl peptidase IV Chains: A,B EC no.: 3.4.14.5
Authors	**Thoma, R., Loeffler, B., Stihle, M., Huber, W., Ruf, A., Hennig, M.**

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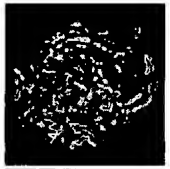
☑ **2OGZ** **Crystal structure of DPP-IV complexed with Lilly aryl ketone inhibitor**



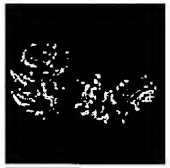
Characteristics **Release Date:** 06-Mar-2007 **Exp. Method:** X Ray Diffraction
Resolution: 2.10 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase Fragment: DPP-IV extracellular domain, residues 39-766 Chains: A,B EC no.: 3.4.14.5

Authors **Sheehan, S.M., Mest, H.J., Watson, B.M., Klimkowski, V.J., Timm, D.E., Cauvin, A., Parson S.H.**

☑ **2BGR** **CRYSTAL STRUCTURE OF HIV-1 TAT DERIVED NONAPEPTIDES TAT(1-9) BOUND TO THE ACTIVE SITE OF DIPEPTIDYL PEPTIDASE IV (CD26)**



Characteristics **Release Date:** 27-Jan-2005 **Exp. Method:** X Ray Diffraction
Resolution: 2.00 Å

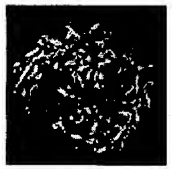
Classification **Hydrolase/complex**

Compound Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE IV Fragment: EXTRACELLULAR DOMAIN, RESIDUES 29-766 Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE Chains: Y,Z
Polymer: 3 Molecule: SUGAR (3-MER)
Polymer: 5 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (3-MER)
Polymer: 7 Molecule: SUGAR (2-MER)

Authors **Weihofen, W.A., Liu, J., Reutter, W., Saenger, W., Fan, H.**

☑ **2GBF** **rat dpp-IV with alkynyl cyanopyrrolidine #1**

Release Date: 04-Jul-2006 **Exp. Method:** X Ray Diffraction



Characteristics **Resolution:** 3.10 Å

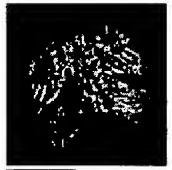
Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Chains: A,B EC no.: 3.4.14.5

Authors **Longenecker, K.L., Stewart, K.D., Madar, D.J., Jakob, C.G., Fry, E.H., Wilk, S., Lin, C.W., Ballaron, S.J., Stashko, M.A., Lubben, T.H., Yong, H., Pireh, D., Pei, Z., Basha, F., Wiedeman, P.E., Von Geldern, T.W., Trevillyan, J.M., Stoll, V.S.**

☑ **1PFQ**

crystal structure of human apo dipeptidyl peptidase IV / CD26



Characteristics **Release Date:** 01-Jul-2003 **Exp. Method:** X Ray Diffraction

Resolution: 1.90 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase IV soluble form Chains: A,B EC no.: 3.4.14.5

Authors **Oefner, C., D`Arcy, A., Mac Sweeney, A., Pierau, S., Gardiner, R., Dale, G.E.**

☑ **2FJP**

Human dipeptidyl peptidase IV/CD26 in complex with an inhibitor

Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.40 Å

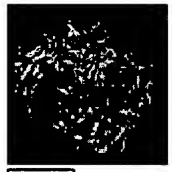
Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: EXTRACELLULAR DOMAIN
Mutation: Ser39Thr Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: 6-(4-{(1S,2S)-2-ammonio-1-[(dimethylamino)carbonyl]-3-[(3S)-3-fluoropyrrolidi 1-yl]-3-oxopropyl}phenyl)[1,2,4]triazolo[1,5-a]pyridin-1-ium bis(trifluoroacetate)

Authors **Edmondson, S.D., Mastracchio, A., Mathvink, R.J., He, J., Harper, B., Park, Y.J., Beconi, M., Di Salvo, J., Eiermann, G.J., He, H., Leiting, B., Leone, J.F., Levorse, D.A., Lyons, K., Patel, R.A., Patel, S.B., Petrov, A., Scapin, G., Shang, J., Roy, R.S., Smith, A., Wu, J.K., Xu, S., Zhu, B., Thornberry, N.A., Weber, A.E.**

☑ **2OAE**

Crystal structure of rat dipeptidyl peptidase (DPPIV) with thiazole-based peptide mimetic #31



Characteristics **Release Date:** 27-Feb-2007 **Exp. Method:** X Ray Diffraction

Resolution: 3.00 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Soluble form: Residues 37-767 Chains: A,B

Compound EC no.: 3.4.14.5

Authors **Backes, B.J., Longenecker, K., Hamilton, G.L., Stewart, K., Lai, C., Kopecka, H., von Gelde T.W., Madar, D.J., Pei, Z., Lubben, T.H., Zinker, B.A., Tian, Z., Ballaron, S.J., Stashko, M.A., Mika, A.K., Beno, D.W., Kempf-Grote, A.J., Black-Schaefer, C., Sham, H.L., Trevillyai J.M.**

☑ **2G5T**

Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 21ag

Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction

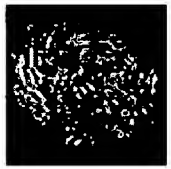
Resolution: 2.30 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl peptidase 4 soluble form Chains: A,B EC no.: 3.4.14.5

Authors **Pei, Z., Li, X., Longenecker, K., Von Geldern, T.W., Wiedeman, P.E., Lubben, T.H., Zinker, B.A., Stewart, K., Ballaron, S.J., Stashko, M.A., Mika, A.K., Beno, D.W., Long, M., Wells, H., Kempf-Grote, A.J., Madar, D.J., McDermott, T.S., Bhagavatula, L., Fickes, M.G., Pireh, D., Solomon, L.R., Lake, M.R., Edalji, R., Fry, E.H., Sham, H.L., Trevillyan, J.M.**

☑ **2G5P**



Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 21ac

Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.40 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl peptidase 4 soluble form Chains: A,B EC no.: 3.4.14.5

Authors **Pei, Z., Li, X., Longenecker, K., Von Geldern, T.W., Wiedeman, P.E., Lubben, T.H., Zinker, B.A., Stewart, K., Ballaron, S.J., Stashko, M.A., Mika, A.K., Beno, D.W., Long, M., Wells, H., Kempf-Grote, A.J., Madar, D.J., McDermott, T.S., Bhagavatula, L., Fickes, M.G., Pireh, D., Solomon, L.R., Lake, M.R., Edalji, R., Fry, E.H., Sham, H.L., Trevillyan, J.M.**

☑ **1WCY**

Crystal Structure Of Human Dipeptidyl Peptidase IV (DPPIV) Complex With Diprotin A

Characteristics **Release Date:** 07-May-2005 **Exp. Method:** X Ray Diffraction

Resolution: 2.20 Å

Classification **Hydrolase**

Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: residues 33-772 Chains: A,B EC no.: 3.4.14.5

Compound	Polymer: 2 Molecule: Diprotin A Chains: C,D Polymer: 3 Molecule: SUGAR (2-MER) Polymer: 5 Molecule: SUGAR (2-MER)
Authors	**Hiramatsu, H., Yamamoto, A., Kyono, K., Higashiyama, Y., Fukushima, C., Shima, H., Sugiyama, S., Inaka, K., Shimizu, R.**

☑ **1X70**

HUMAN DIPEPTIDYL PEPTIDASE IV IN COMPLEX WITH A BETA AMINO ACID INHIBITOR

Characteristics	**Release Date:** 18-Jan-2005 **Exp. Method:** X Ray Diffraction **Resolution:** 2.10 Å
Classification	**Hydrolase**
Compound	Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: extracellular domain Mutation: S39T Chains: A,B EC no.: 3.4.14.5 Polymer: 2 Molecule: SUGAR (NAG-NAG) Polymer: 4 Molecule: SUGAR (NAG-NAG) Polymer: 5 Molecule: SUGAR (NAG-NAG) Polymer: 6 Molecule: SUGAR (NAG-NAG) Polymer: 7 Molecule: SUGAR (NAG-NAG) Polymer: 8 Molecule: SUGAR (NAG-NAG) Polymer: 9 Molecule: SUGAR (NAG-NAG) Polymer: 10 Molecule: SUGAR (NAG-NAG) Polymer: 11 Molecule: SUGAR (NAG-NAG)
Authors	**Kim, D., Wang, L., Beconi, M., Eiermann, G.J., Fisher, M.H., He, H., Hickey, G.J., Kowalchi J.E., Leiting, B., Lyons, K., Marsilio, F., McCann, M.E., Patel, R.A., Petrov, A., Scapin, G., Patel, S.B., Roy, R.S., Wu, J.K., Wyvratt, M.J., Zhang, B.B., Zhu, L., Thornberry, N.A., Weber, A.E.**

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2I03 **Crystal structure of human dipeptidyl peptidase 4 (DPP IV) with potent alkynyl cyanopyrrolidine (ABT-279)**

Characteristics **Release Date:** 12-Dec-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.40 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Chains: A,B,C,D EC no.: 3.4.14.5

Authors **Madar, D.J., Kopecka, H., Pireh, D., Yong, H., Pei, Z., Li, X., Wiedeman, P.E., Djuric, S.W., Von Geldern, T.W., Fickes, M.G., Bhagavatula, L., McDermott, T., Wittenberger, S., Richards, S.J., Longenecker, K.L., Stewart, K.D., Lubben, T.H., Ballaron, S.J., Stashko, M.A., Long, M.A., Wells, H., Zinker, B.A., Mika, A.K., Beno, D.W., Kempf-Grote, A.J., Polakowski, J., Segreti, J., Reinhart, G.A., Fryer, R.M., Sham, H.L., Trevillyan, J.M.**

1TK3 **Crystal Structure Of Human Apo Dipeptidyl Peptidase IV/CD26**

Characteristics **Release Date:** 06-Jul-2004 **Exp. Method:** X Ray Diffraction

Resolution: 2.00 Å

Classification **Hydrolase**

Compound
Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: Extracellular domain Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: SUGAR (3-MER)
Polymer: 3 Molecule: SUGAR (3-MER)
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 5 Molecule: SUGAR (3-MER)
Polymer: 6 Molecule: SUGAR (2-MER)
Polymer: 7 Molecule: SUGAR (2-MER)
Polymer: 9 Molecule: SUGAR (3-MER)
Polymer: 10 Molecule: SUGAR (2-MER)
Polymer: 11 Molecule: SUGAR (3-MER)
Polymer: 12 Molecule: SUGAR (3-MER)

Polymer: 13 Molecule: SUGAR (2-MER)

Authors **Bjelke, J.R., Christensen, J., Branner, S., Wagtmann, N., Olsen, C., Kanstrup, A.B., Rasmussen, H.B.**

☑ **1TKR** **Human Dipeptidyl Peptidase IV/CD26 inhibited with Diisopropyl FluoroPhosphate**

Characteristics **Release Date:** 06-Jul-2004 **Exp. Method:** X Ray Diffraction

Resolution: 2.70 Å

Classification **Hydrolase**

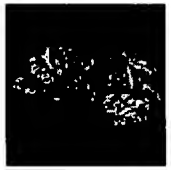
Compound

Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: Extracellular domain Chains: A,B EC no.: 3.4.14.5

Polymer: 2 Molecule: SUGAR (3-MER)
Polymer: 3 Molecule: SUGAR (3-MER)
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 5 Molecule: SUGAR (3-MER)
Polymer: 6 Molecule: SUGAR (2-MER)
Polymer: 7 Molecule: SUGAR (2-MER)
Polymer: 8 Molecule: SUGAR (2-MER)
Polymer: 10 Molecule: SUGAR (2-MER)
Polymer: 11 Molecule: SUGAR (3-MER)
Polymer: 12 Molecule: SUGAR (3-MER)
Polymer: 13 Molecule: SUGAR (2-MER)

Authors **Bjelke, J.R., Christensen, J., Branner, S., Wagtmann, N., Olsen, C., Kanstrup, A.B., Rasmussen, H.B.**

☑ **1U8E** **HUMAN DIPEPTIDYL PEPTIDASE IV/CD26 MUTANT Y547F**



Characteristics **Release Date:** 17-Aug-2004 **Exp. Method:** X Ray Diffraction

Resolution: 2.20 Å

Classification **Hydrolase**

Compound

Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: EXTRACELLULAR DOMAIN Mutation: Y547F Chains: A,B EC no.: 3.4.14.5

Polymer: 2 Molecule: SUGAR (3-MER)
Polymer: 3 Molecule: SUGAR (3-MER)
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 5 Molecule: SUGAR (3-MER)
Polymer: 6 Molecule: SUGAR (2-MER)
Polymer: 7 Molecule: SUGAR (2-MER)
Polymer: 9 Molecule: SUGAR (3-MER)
Polymer: 10 Molecule: SUGAR (2-MER)

Polymer: 11 Molecule: SUGAR (3-MER)
Polymer: 12 Molecule: SUGAR (3-MER)
Polymer: 13 Molecule: SUGAR (2-MER)

Authors **BJELKE, J.R., CHRISTENSEN, J., BRANNER, S., WAGTMANN, N., OLSEN, C., KANSTRUP, A.B., RASMUSSEN, H.B.**

☑ **2BUA**

CRYSTAL STRUCTURE OF PORCINE DIPEPTIDYL PEPTIDASE IV (CD26) IN COMPLEX WITH A LOW MOLECULAR WEIGHT INHIBITOR.

Characteristics **Release Date:** 23-Jan-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.56 Å

Classification **Complex (hydrolase/inhibitor)**

Compound Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE IV Fragment: EXTRACELLULAR DOMAIN, RESIDUES 39-766 Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 3 Molecule: SUGAR (2-MER)

Authors **Nordhoff, S., Cerezo-Galvez, S., Feurer, A., Hill, O., Matassa, V.G., Metz, G., Rummey, C., Thiemann, M., Edwards, P.J.**

☑ **2BUC**

CRYSTAL STRUCTURE OF PORCINE DIPEPTIDYL PEPTIDASE IV (CD26) IN COMPLEX WITH A TETRAHYDROISOQUINOLINE INHIBITOR

Characteristics **Release Date:** 23-Jan-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.50 Å

Classification **Complex (hydrolase/inhibitor)**

Compound Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE IV Fragment: EXTRACELLULAR DOMAIN, RESIDUES 39-766 Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 3 Molecule: SUGAR (2-MER)
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (2-MER)

Authors **Nordhoff, S., Cerezo-Galvez, S., Feurer, A., Hill, O., Matassa, V.G., Metz, G., Rummey, C., Thiemann, M., Edwards, P.J.**

☑ **1J2E**

Crystal structure of Human Dipeptidyl peptidase IV

Characteristics **Release Date:** 30-Dec-2003 **Exp. Method:** X Ray Diffraction
Resolution: 2.60 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase IV Fragment: residues 33-772 Chains: A,B EC

no.: 3.4.14.5

Authors **Hiramatsu, H., Kyono, K., Higashiyama, Y., Fukushima, C., Shima, H., Sugiyama, S., Inaka K., Yamamoto, A., Shimizu, R.**

☑ **2BGN**

HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE TRP2-TAT (1-9) BOUND TO THE ACTIVE SITE OF DIPEPTIDYL PEPTIDASE IV (CD26)

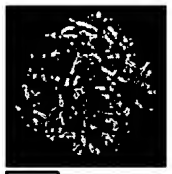
Characteristics **Release Date:** 27-Jan-2005 **Exp. Method:** X Ray Diffraction
Resolution: 3.15 Å

Classification **Hydrolase/complex**

Compound
Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE IV Fragment: EXTRACELLULAR DOMAIN, RESIDUES 39-766 Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 2 Molecule: ADENOSINE DEAMINASE Chains: E,F,G,H EC no.: 3.5.4.4
Polymer: 3 Molecule: TAT PROTEIN Fragment: HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE, RESIDUES 1-9 Mutation: YES Chains: W,X,Y,Z Other Details: ASP2TRP VARIAI OF HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE
Polymer: 4 Molecule: SUGAR (3-MER)
Polymer: 5 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (4-MER)
Polymer: 8 Molecule: SUGAR (2-MER)

Authors **Weihofen, W.A., Liu, J., Reutter, W., Saenger, W., Fan, H.**

☑ **1NU8**



Crystal structure of human dipeptidyl peptidase IV (DPP-IV) in complex with Diprotin A (ILI)

Characteristics **Release Date:** 26-Aug-2003 **Exp. Method:** X Ray Diffraction
Resolution: 2.50 Å

Classification **Hydrolase**

Compound
Polymer: 1 Molecule: Dipeptidyl peptidase IV Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: 3-mer peptide Chains: D

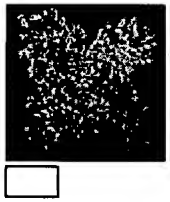
Authors **Thoma, R., Loeffler, B., Stihle, M., Huber, W., Ruf, A., Hennig, M.**

☑ **1W1I**

CRYSTAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV (DPPIV OR CD26) IN COMPLEX WITH ADENOSINE DEAMINASE

Characteristics **Release Date:** 02-Sep-2004 **Exp. Method:** X Ray Diffraction
Resolution: 3.03 Å

Classification **Hydrolase/complex**



Compound

Polymer: 1 Molecule: DIPEPTIDYL PEPTIDASE IV Fragment: EXTRACELLULAR DOMAIN 39 - 76(
Chains: A,B,C,D EC no.: 3.4.14.5

Polymer: 2 Molecule: ADENOSINE DEAMINASE Chains: E,F,G,H EC no.: 3.5.4.4
Polymer: 3 Molecule: SUGAR (3-MER)
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 5 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (4-MER)
Polymer: 8 Molecule: SUGAR (2-MER)
Polymer: 9 Molecule: SUGAR (2-MER)
Polymer: 10 Molecule: SUGAR (4-MER)
Polymer: 11 Molecule: SUGAR (2-MER)
Polymer: 12 Molecule: SUGAR (3-MER)
Polymer: 13 Molecule: SUGAR (2-MER)
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Polymer: 18 Molecule: SUGAR (2-MER)
Polymer: 19 Molecule: SUGAR (4-MER)
Polymer: 20 Molecule: SUGAR (2-MER)

Authors **Weihofen, W.A., Liu, J., Reutter, W., Saenger, W., Fan, H.**

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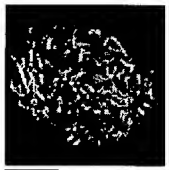
☑ **2AJL**



X-ray Structure of Novel Biaryl-Based Dipeptidyl peptidase IV inhibitor

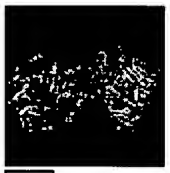
Characteristics **Release Date:** 08-Nov-2005 **Exp. Method:** X Ray Diffraction
Resolution: 2.50 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl peptidase 4 soluble form, residue: 39-766 Chains: I,J EC no.: 3.4.14.5

Authors **Qiao, L., Baumann, C.A., Crysler, C.S., Ninan, N.S., Abad, M.C., Spurlino, J.C., Desjarlais, R.L., Kervinen, J., Neeper, M.P., Bayoumy, S.S., Williams, R., Deckman, I.C., Dasgupta, M., Reed, R.L., Huebert, N.D., Tomczuk, B.E., Moriarty, K.J.**

☑ **1R9N**



Crystal Structure of human dipeptidyl peptidase IV in complex with a decapeptide (tNPY) at 2.3 Ang. Resolution

Characteristics **Release Date:** 29-Mar-2005 **Exp. Method:** X Ray Diffraction
Resolution: 2.30 Å

Classification **Hydrolase**

Compound
Polymer: 1 Molecule: Dipeptidyl peptidase IV Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 2 Molecule: Neuropeptide Y Chains: E,F,G,H
Polymer: 4 Molecule: SUGAR (2-MER)
Polymer: 5 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (2-MER)
Polymer: 7 Molecule: SUGAR (2-MER)

Authors **Aertgeerts, K., Ye, S., Tennant, M.G., Kraus, M.L., Rogers, J., Sang, B.-C., Skene, R.J., We D.R., Prasad, G.S.**

☑ **2AJC**

Porcine dipeptidyl peptidase IV (CD26) in complex with 4-(2-Aminoethyl)-benzene sulphonyl fluoride (AEBSF)

Characteristics **Release Date:** 28-Feb-2006 **Exp. Method:** X Ray Diffraction
Resolution: 1.95 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Extracellular domain Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 3 Molecule: SUGAR (2-MER)
Polymer: 4 Molecule: SUGAR (3-MER)

Authors **Engel, M., Hoffmann, T., Manhart, S., Heiser, U., Chambre, S., Huber, R., Demuth, H.U., Bode, W.**

☑ **1R9M**

Crystal Structure of Human Dipeptidyl Peptidase IV at 2.1 Ang. Resolution.

Characteristics **Release Date:** 29-Jun-2004 **Exp. Method:** X Ray Diffraction
Resolution: 2.10 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase IV Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 3 Molecule: SUGAR (2-MER)
Polymer: 4 Molecule: SUGAR (3-MER)
Polymer: 5 Molecule: SUGAR (2-MER)
Polymer: 6 Molecule: SUGAR (2-MER)
Polymer: 8 Molecule: SUGAR (2-MER)
Polymer: 9 Molecule: SUGAR (2-MER)
Polymer: 10 Molecule: SUGAR (4-MER)
Polymer: 11 Molecule: SUGAR (2-MER)

Authors **Aertgeerts, K., Ye, S., Tennant, M.G., Kraus, M.L., Rogers, J., Sang, B.C., Skene, R.J., Web D.R., Prasad, G.S.**

☑ **2AJD**

Porcine dipeptidyl peptidase IV (CD26) in complex with L-Pro-boro-L-Pro (boroPro)

Characteristics **Release Date:** 28-Feb-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.56 Å

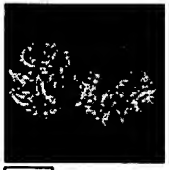
Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Extracellular domain Chains: A,B,C,D EC no.: 3.4.14.5
Polymer: 3 Molecule: SUGAR (2-MER)
Polymer: 4 Molecule: SUGAR (3-MER)

Authors **Engel, M., Hoffmann, T., Manhart, S., Heiser, U., Chambre, S., Huber, R., Demuth,**

H.U., Bode, W.

☑ 2IIT



Human dipeptidyl peptidase 4 in complex with a diazepan-2-one inhibitor

Characteristics **Release Date:** 28-Nov-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.35 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 soluble form Fragment: EXTRACELLULAR DOMAIN (residues 39-766) Mutation: Ser39Thr Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: SUGAR (2-MER)

Authors **Biftu, T., Feng, D., Qian, X., Liang, G.B., Kieczykowski, G., Eiermann, G., He, H., Leiting, B., Lyons, K., Petrov, A., Sinha-Roy, R., Zhang, B., Scapin, G., Patel, S., Gao, Y.D., Singh, S., Wu, J., Zhang, X., Thornberry, N.A., Weber, A.E.**

☑ 2IIV

Human dipeptidyl peptidase 4 in complex with a diazepan-2-one inhibitor

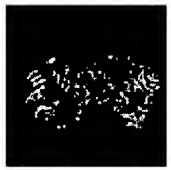
Characteristics **Release Date:** 28-Nov-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.15 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 soluble form Fragment: EXTRACELLULAR DOMAIN (residues 39-766) Mutation: Ser39Thr Chains: A,B EC no.: 3.4.14.5
Polymer: 2 Molecule: SUGAR (2-MER)

Authors **Biftu, T., Feng, D., Qian, X., Liang, G.B., Kieczykowski, G., Eiermann, G., He, H., Leiting, B., Lyons, K., Petrov, A., Sinha-Roy, R., Zhang, B., Scapin, G., Patel, S., Gao, Y.D., Singh, S., Wu, J., Zhang, X., Thornberry, N.A., Weber, A.E.**

☑ 2G63



Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 24b

Characteristics **Release Date:** 04-Jul-2006 **Exp. Method:** X Ray Diffraction
Resolution: 2.00 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Dipeptidyl peptidase 4 soluble form Chains: A,B,C,D EC no.: 3.4.14.5

Authors **Pei, Z., Li, X., Longenecker, K., Von Geldern, T.W., Wiedeman, P.E., Lubben, T.H., Zinker, B.A., Stewart, K., Ballaron, S.J., Stashko, M.A., Mika, A.K., Beno, D.W., Long, M., Wells, H., Kempf-Grote, A.J., Madar, D.J., McDermott, T.S., Bhagavatula, L., Fickes, M.G., Pireh, D., Solomon, L.R., Lake, M.R., Edalji, R., Fry, E.H., Sham, H.L., Trevillyan, J.M.**

☑ **1N1M**

Human Dipeptidyl Peptidase IV/CD26 in complex with an inhibitor

Characteristics **Release Date:** 27-Dec-2002 **Exp. Method:** X Ray Diffraction

Resolution: 2.50 Å

Classification **Hydrolase**

Compound

Polymer: 1 Molecule: Dipeptidyl peptidase IV SOLUBLE FORM Fragment: Extracellular domain Chains: A,B EC no.: 3.4.14.5 (EC)
Polymer: 2 Molecule: NAG-NAG-FUC
Polymer: 3 Molecule: NAG-NAG-FUC
Polymer: 4 Molecule: NAG-NAG
Polymer: 5 Molecule: NAG-NAG-MAN
Polymer: 6 Molecule: NAG-NAG
Polymer: 7 Molecule: NAG-NAG
Polymer: 9 Molecule: NAG-FUC
Polymer: 10 Molecule: NAG-NAG
Polymer: 11 Molecule: NAG-NAG-MAN
Polymer: 12 Molecule: NAG-NAG-MAN
Polymer: 13 Molecule: NAG-NAG

Authors **Rasmussen, H.B., Branner, S., Wiberg, F.C., Wagtmann, N.R.**

☑ **2AJ8**

Porcine dipeptidyl peptidase IV (CD26) in complex with 7-Benzyl-1,3-dimethyl-8-piperazin-1-yl-3,7-dihydro-purine-2,6-dione (BDPX)

Characteristics **Release Date:** 28-Feb-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.11 Å

Classification **Hydrolase**

Compound

Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Extracellular domain Chains: A,B,C,D EC no.: 3.4.14.5 (EC)
Polymer: 3 Molecule: SUGAR (2-MER)
Polymer: 4 Molecule: SUGAR (3-MER)

Authors **Engel, M., Hoffmann, T., Manhart, S., Heiser, U., Chambre, S., Huber, R., Demuth, H.U., Bode, W.**

1 2 3 4 5

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Porcine dipeptidyl peptidase IV (CD26) in complex with the tripeptide tert-butyl-Gly-L-Pro-L-Ile (tBu-GPI)

Characteristics **Release Date:** 28-Feb-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.75 Å

Classification **Hydrolase**

Compound Polymer: 1 Molecule: Dipeptidyl peptidase 4 Fragment: Extracellular domain Chains: A,B,C,D EC no.: 3.4.14.5

Polymer: 2 Molecule: TERT-BUTYL-GLY-PRO-ILE (tBu-GPI) Chains: I,J,K,L

Polymer: 4 Molecule: SUGAR (2-MER)

Polymer: 5 Molecule: SUGAR (3-MER)

Authors **Engel, M., Hoffmann, T., Manhart, S., Heiser, U., Chambre, S., Huber, R., Demuth, H.U., Bode, W.**